COLLECTION OF SIMULATED XRD POWDER PATTERNS FOR ZEOLITES

M.M.J. Treacy
and
J.B. Higgins

Fourth Revised Edition
2001

Published on behalf of the
Structure Commission of the International Zeolite Association

ELSEVIER

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PREFACE

The synthesis and characterization of new zeolite materials continues unabated. The IZA Structure Commission has recognized thirty-five new topologies since the 3rd edition of this *Collection* was prepared in 1995. The total number of zeolite structure refinements has surpassed 3000 with over 1000 new refinements since 1995. Not surprisingly, the most scrutinized framework topology is that of faujasite, **FAU**, with about 600 structural studies. Probably no other inorganic host structure has received such attention. With these numbers it is apparent that this *Collection* is not comprehensive. The scope of the *Collection* has been broadly defined to include materials of interest to zeolite scientists, following the policies established at recent IZA conferences. We have attempted to be as inclusive as possible to give the users of this publication the maximum information. The structures of the porous solids that we considered comprise corner-sharing tetrahedra, and are not limited to a specific chemical composition. Materials such as metal phosphates and silica polymorphs are included.

The present *Collection* serves as a source of reference patterns for pure zeolite phases. The data will be helpful in establishing the structural purity of experimental phases and in indexing their diffraction patterns. The data will also aid in the determination of changes in the lattice parameters with changing composition, assessing preferred orientation effects, background evaluation, and line broadening. We have also included diffraction patterns of several common dense silicate phases to facilitate their detection in mixed phase syntheses.

The numerical data comprises 2θ values for CuKα radiation ($\lambda = 1.5418$ Å), d-spacings, relative intensities, hkl Miller indices and multiplicity, M_{hkl}. Data representing 133 framework topologies have been included in this *Collection*. In most cases, X-ray or neutron refinements of hydrated or as-synthesized forms are used.

This edition differs significantly from the 1996 3rd edition which included atomic coordinates. Because of space constraints coordinate data has not been included in this edition, but are available in electronic form, along with the complete contents of this edition, at:

http://www.iza-structure.org/databases/

This web site also contains an interactive powder pattern calculator that allows the user to change the input and variables for a powder pattern calculation.

This book was typeset using LaTeX with the standard computer modern typeface. The LaTeX file, and associated postscript plots, were generated using a C program written by M. M. J. Treacy.

We wish to acknowledge the assistance and collaboration of the members of the IZA Structure Commission in proofreading the manuscript and for providing additional information. We are indebted to our companies (NEC Research Institute, Inc., and Air Products and Chemicals, Inc.) for support of this project. We are grateful to Peggy Bisher for keeping the reference data files impeccably organized. Finally, we acknowledge the patience and support of our wives Laura and Carol.

Michael M. J. Treacy, Princeton, NJ
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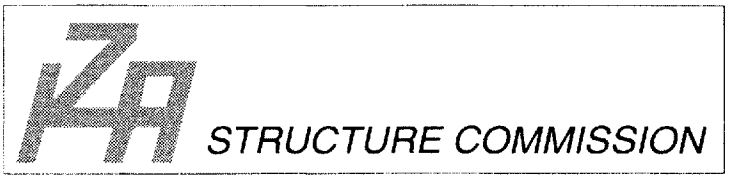
January 2001



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Additional IZA publications:

Atlas of Zeolite Framework Types, 5th revised edition (2001),
Ch. Baerlocher, W. M. Meier and D. H. Olson.

Compilation of Extra Framework Sites in Zeolites (1982),
W. J. Mortier. (out of print)

Verified Syntheses of Zeolitic Materials, 2nd revised edition (2001),
H. Robson, editor; and K. P. Lillerud, XRD patterns.

See also: http://www.iza-online.org/

EXPLANATORY NOTES

The numerical data and the simulated powder patterns presented in this *Collection* are to a great extent self-explanatory. In order to facilitate the use of these reference patterns some pertinent remarks regarding the keywords used in the data section are summarized below. The input structural data have been deposited on the worldwide web at:

http://www.iza-structure.org/databases/

This *Collection*, including updates, will be accessible at the above address.

ZEOLITE FRAMEWORK TYPES

The three-letter framework type codes, recognized by the IUPAC Commission on Zeolite Nomenclature, have been used to organize the entries in this publication. The powder diffraction data and simulated patterns for the reference structures are listed alphabetically according to the respective framework type code. An index of material names, and associated three-letter codes, is included in the companion volume, the *Atlas of Zeolite Framework Types* (Baerlocher, Meier and Olson (2001)).

COMPOSITION

Compositions are expressed in terms of the full unit cell content. Two compositions are provided. The CHEMICAL COMPOSITION is the nominal material composition provided in the original reference, and is usually obtained from chemical analysis. The REFINED COMPOSITION is derived from the structure refinement. Because of the complexities of structure refinements, the chemical and refined compositions do not always concur. When available, refinements of hydrated zeolites were used to calculate the patterns. For synthetic zeolites, if the zeolite had been synthesized in the presence of organic material, those refinements of the uncalcined products that contained the occluded organic molecules were chosen. The sample locality is given in the case of natural zeolites.

CRYSTAL DATA

Crystal data includes lattice parameters and space group information from the International Tables for Crystallography, 4th revised edition 1995, and incorporates the new *e* 'double-glide' plane. Consequently, some space group symbols will differ from those listed in the original references. Two entries in this *Collection* are affected by this change; EU-1 (**EUO**) which has space group symbol *Cmme* (formerly *Cmma*), and gottardiite (**NES**) which has space group symbol *Cmce* (formerly *Cmca*). The type of refinement, along with the final *R*-values, is listed with the unit cell parameters.

REFERENCE

Reference cites the literature from which the crystal data, atomic coordinates, and temperature factors were obtained. In many cases there are multiple refinements of the same zeolitic material, but because of space limitations not all refinements could be included. We would be appreciative if

authors and users would inform us of any errors or omissions. A listing of the references for isotypic species can be found in the *Atlas of Zeolite Framework Types* (Baerlocher, Meier and Olson (2001)). A list of references to structure analyses of zeolites with different cations, up to 1982, is given in the *Compilation of Extra Framework Sites in Zeolites*, W. J. Mortier (1982).

POWDER PATTERN IDENTIFICATION TABLE

A table is provided to assist in the identification of powder patterns of unknown materials. The 2θ (°) values of the three most pronounced low-angle reflections are listed. Usually, these reflections are simply the three strongest peaks. In many instances, a pronounced low-angle reflection will be included, even if it is not among the most intense. In the 3rd edition (1996) of the *Collection* this table was assembled by visual inspection of the computed powder patterns. For this fourth edition (2001) of the *Collection*, the table was generated automatically from the computed diffraction patterns. To achieve good correspondence with the hand-generated table of the 3rd (1996) edition of the *Collection*, a peak intensity weighting function $W(2\theta)$ was used

$$W(2\theta) = 1 + A \exp\left[-(2\theta)^2/2\sigma^2\right]. \tag{1}$$

The parameters were set to $A = 10$, and $\sigma = 7°$. This function is strongly weighted towards the low angle peaks, particularly those below about 10°, which, even if relatively weak, tend to offer a more characteristic fingerprint of a material compared to the abundance of strong peaks that tend to cluster around 25° in most zeolitic materials.

The data for all the materials presented in this work are sorted by increasing 2θ value in the table. To identify an unknown material, measure the 2θ values of the three most pronounced peaks (assigning strong weighting to any pronounced low-angle peaks, particularly those below about 10°) and find those materials with corresponding reflections at those values. This provides a starting point for a more detailed comparison of the experimental and calculated patterns.

CALCULATED POWDER DIFFRACTION DATA

The powder diffraction data include the 2θ-values for CuKα radiation, d-spacings, relative intensities $I_{\rm rel}$, Miller indices hkl and multiplicity M_{hkl}, for the strongest 135 reflections with an integrated intensity $I_{\rm rel}$ greater than 0.1. The strongest reflection is set to $I_{\rm rel} = 100$. The scattering factors used for the framework T- and O-atoms in the structure factor computations were those selected by the authors of the original work. If none had been specified, we chose atomic (neutral) scattering factors. No adsorption corrections were applied to the data, and anisotropic temperature factors were converted to isotropic temperature factors $B_{\rm iso}$ (Å^2) using equations reported by W. C. Hamilton, *Acta Cryst.*, **12** 609–610 (1959).

Materials with the same framework type code (i.e. framework topology) may have very different diffraction patterns, so for some framework type codes several different reference materials have been included. Examples listed under **FAU**, **GIS**, **MFI** and **NAT** illustrate the extent of the differences observed in the diffraction patterns of materials with identical framework topologies but

variations in composition and/or symmetry.

SIMULATED POWDER PATTERNS

The powder patterns for CuKα radiation are reproduced from 0° to 50° 2θ. The patterns, and associated tables, were calculated using a custom C program written by M. M. J. Treacy. The intensity scale is kept variable to accommodate extreme situations. The intensity range is usually plotted between 0 and I_{max} = 100. If only one or a few peaks are very intense, and the rest of the pattern consists of low-intensity reflections, I_{max} is set at a lower value (see ordinate) to show sufficient detail in the low-intensity region of the pattern. The scale of the ordinate is always calibrated in percent relative intensity of the maximum peak height. Frequently, the peak intensities in the plots will not be identical to the integrated intensities listed in the corresponding tables, because of the possibility of overlapping diffraction peaks. A Lorentzian profile was assumed for the calculation of the pattern. The full width at half maximum (FWHM) of all peaks was set to be 0.08° 2θ. Many real samples will in general give diffraction patterns with broader lines due to instrumental broadening, disorder, or small crystallite size. However, synchrotron powder diffraction data of some zeolite materials exhibit FWHM of less than 0.04° 2θ.

Because hydrated forms of natural zeolites or as-synthesized forms were used whenever refined atomic parameters were available, the plots should be easily comparable to experimental patterns. In some cases, only structure refinements of dehydrated or calcined forms were available. Significant differences in the intensities of low-angle peaks may be found when comparing the calculated pattern to experimental patterns of hydrated or as-synthesized materials.

Finally, a note of caution. The patterns are useful in helping to establish the structural purity of a zeolite phase, yet they may not always allow one to readily and unambiguously determine the framework type of the sample. This assignment is often not straightforward and may require more sophisticated analyses. W. J. Rohrbaugh and E. W. Wu review the factors affecting the diffraction characteristics of zeolite materials (ACS Symposium Series **411** 279–302 (1989)).

POWDER PATTERN SIMULATIONS OF DISORDERED INTERGROWTHS

A number of zeolitic materials crystallize as disordered planar intergrowths of "end-member" frameworks. Two of the better-studied series are the **FAU/EMT** intergrowths (such as ZSM-2, ZSM-3, ZSM-20, ECR-30, CSZ-1 and CSZ-3) and the intergrown zeolite beta and its natural analog tschernichite. Powder patterns for five of the more commonly observed coherently intergrown series were calculated using the DIFFaX computer program (M. M. J. Treacy, J. M. Newsam and M. W. Deem, *Proc. R. Soc. Lond.* A **433** 499–520 (1991)). Random stacking faults are assumed. The five series are; the beta family; SSZ-33/SSZ-26; **FAU/EMT**; **MFI/MEL**; and **OFF/ERI**. The stacking fault probability is incremented from 0 to 1 in steps of 0.1. Stacking fault probabilities of 0 and 1 represent the unfaulted end-members.

Additional information on disordered intergrowths can be found in the *Catalog of Disordered Zeolite Structures*, which is available electronically at http://www.iza-structure.org/databases/.

CHANGES SINCE THE THIRD REVISED EDITION

- 35 new framework types have been approved since the third revised edition, and are included in this fourth revised edition. The new framework types are:

ACO	**AEN**	**AFN**	**ASV**	**AWO**	**CFI**	**CGF**
CGS	**CZP**	**DFT**	**DON**	**ESV**	**FRA**	**GON**
IFR	**ISV**	**ITE**	**MSO**	**MTF**	**MWW**	**OSI**
OSO	**SAO**	**SAS**	**SAT**	**SAV**	**SBE**	**SBS**
SBT	**SFE**	**SFF**	**STF**	**STT**	**TER**	**TSC**

- Due to space constraints, the refined structure coordinates are not listed in the printed version of this *Collection*. An electronic PDF version of this *Collection*, complete with coordinates, can be found at:

http://www.iza-structure.org/databases/

- Errors in the space group settings of Maricopaite (**MOR**) and chiavennite (**-CHI**) have been fixed. These corrections change the diffraction patterns and the listed peak intensities.
- The distance least squares refinement of liottite (**LIO**), given in the third revised edition, has been replaced by a single crystal x-ray refinement.
- The entry for Na-exchanged K-F (**EDI**) has been removed due to inconsistencies in the refinement.
- A typographic error in the published coordinates for perlialite (**LTL**) has been corrected. This correction has changed the diffraction pattern noticeably.
- An error in the cation occupancies for the mineral faujasite (**FAU**) has been corrected. This correction has changed the diffraction pattern noticeably.
- The refinements of MAPO–39 (**ATN**) and offretite (**OFF**) have been replaced.
- A refinement for low silica zeolite-X (**FAU**) has been added.
- A small number of typographic errors in atom coordinates have been corrected.

POWDER PATTERN IDENTIFICATION TABLE

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Powder Pattern Identification Table

$2\theta^\circ$	Material	Code
3.33	Franzinite	**FRA**
3.42	Cloverite	**-CLO**
3.56	Paulingite	**PAU**
4.14	NaZ-21	**LTN**
4.56	Decamethonium DAF-1	**DFO**
4.80	VPI-9	**VNI**
4.83	Cloverite	**-CLO**
4.84	Tschörtnerite	**TSC**
5.04	Paulingite	**PAU**
5.31	AlPO-8	**AET**
5.38	VPI-5	**VFI**
5.50	Perlialite	**LTL**
5.55	Linde Type L	**LTL**
5.55	Mazzite	**MAZ**
5.59	Tschörtnerite	**TSC**
5.63	UCSB-8Co	**SBE**
5.64	Chiavennite	**-CHI**
5.72	UCSB-6GaCo	**SBS**
5.76	MCM-35	**MTF**
5.87	EMC-2, Calcined	**EMT**
5.87	EMC-2, Partially Dehydrated	**EMT**
5.92	Cloverite	**-CLO**
5.96	Li-LSX	**FAU**
6.02	UCSB-10GaZn	**SBT**
6.04	UTD-1	**DON**
6.10	Na-X, Dehydrated	**FAU**
6.12	Na-X, Hydrated	**FAU**
6.19	Faujasite	**FAU**
6.23	EMC-2, Partially Dehydrated	**EMT**
6.24	EMC-2, Calcined	**EMT**
6.31	Na-Y, Siliceous	**FAU**
6.32	UCSB-10GaZn	**SBT**
6.33	Ultrastable Y, Dehydrated Dealuminated	**FAU**
6.39	Maricopaite	**MOR**
6.41	UCSB-8Co	**SBE**
6.48	1-aminoadamantane Deca-Dodecasil 3R	**DDR**
6.50	UCSB-6GaCo	**SBS**
6.51	Mordenite	**MOR**
6.57	AlPO-8	**AET**
6.57	Di-n-propylamine MAPSO-46	**AFS**
6.58	UCSB-6GaCo	**SBS**
6.58	SSZ-48, Calcined	**SFE**
6.65	EMC-2, Calcined	**EMT**
6.65	EMC-2, Partially Dehydrated	**EMT**
6.69	(Cs,K) ZK5, Dehydrated	**KFI**
6.77	NaZ-21	**LTN**
6.78	VPI-8	**VET**
6.82	UiO-6, Calcined	**OSI**
6.82	Roggianite	**-RON**
6.85	AlPO-41, Calcined	**AFO**
6.88	ITQ-7, Siliceous, Calcined	**ISV**
6.93	CIT-5	**CFI**
6.96	GUS-1	**GON**
6.98	Beta, Polymorph A SiO_2 Framework	***BEA**
7.01	ITQ-7, Siliceous, Calcined	**ISV**
7.04	UCSB-10GaZn	**SBT**
7.05	NU-87	**NES**
7.09	ITQ-1, Calcined (Siliceous MCM-22)	**MWW**
7.10	Beryllophosphate-H	**BPH**
7.18	ITQ-1, Calcined (Siliceous MCM-22)	**MWW**

$2\theta^\circ$	Material	Code
7.18	Linde Type A, Hydrated	**LTA**
7.20	Linde Type A, Dehydrated	**LTA**
7.33	CIT-5	**CFI**
7.40	Terranovaite	**TER**
7.41	N_2, Piperidine Dodecasil 1H	**DOH**
7.42	SAPO-56	**AFX**
7.42	Gmelinite	**GME**
7.43	Boggsite	**BOG**
7.43	Tetrapropylammonium Fluoride AlPO-5	**AFI**
7.47	ZSM-12, Calcined	**MTW**
7.49	MCM-61	**MSO**
7.55	UTD-1	**DON**
7.61	Tetrapropylammonium SAPO-40	**AFR**
7.63	ZSM-12, Calcined	**MTW**
7.66	Offretite	**OFF**
7.66	CIT-1	**CON**
7.67	STA-1, Magnesium Aluminophosphate	**SAO**
7.68	1-aminoadamantane Deca-Dodecasil 3R	**DDR**
7.69	Erionite	**ERI**
7.71	Bellbergite	**EAB**
7.71	Piperidine AlPO-17	**ERI**
7.72	ITQ-7, Siliceous, Calcined	**ISV**
7.72	Di-n-propylamine MAPSO-46	**AFS**
7.72	SSZ-44, Calcined	**SFF**
7.73	ERS-7 Framework	**ESV**
7.74	Beta, Polymorph A SiO_2 Framework	***BEA**
7.75	ZSM-18, SiO_2 Framework	**MEI**
7.78	Ferrierite	**FER**
7.80	Gottardiite	**NES**
7.82	ZSM-57, SiO_2 Framework	**MFS**
7.84	Boggsite	**BOG**
7.84	CIT-1	**CON**
7.88	MAPO-36, Calcined	**ATS**
7.89	Dodecasil 3C	**MTN**
7.90	NU-87	**NES**
7.91	Decamethonium DAF-1	**DFO**
7.92	EU-1, Calcined, Rehydrated	**EUO**
7.93	ZSM-11, Calcined	**MEL**
7.94	NaZ-21	**LTN**
7.94	ZSM-5, Calcined	**MFI**
7.94	Ammonium Fluoride ZSM-23	**MTT**
7.95	Tetrapropylammonium ZSM-5	**MFI**
7.95	2-aminopentane Nonasil	**NON**
7.99	SSZ-35, Calcined	**STF**
8.01	ZSM-5, Calcined	**MFI**
8.01	Di-n-propylamine CoAPO-50	**AFY**
8.01	ITQ-1, Calcined (Siliceous MCM-22)	**MWW**
8.02	AlPO-52, Calcined, Rehydrated	**AFT**
8.06	Tetrapropylammonium SAPO-40	**AFR**
8.06	SSZ-44, Calcined	**SFF**
8.07	SSZ-48, Calcined	**SFE**
8.09	SSZ-35, Calcined	**STF**
8.09	Di-isopropylamine MnAPO-11	**AEL**
8.10	AlPO-11, Calcined	**AEL**
8.11	ERS-7 Framework	**ESV**
8.11	SSZ-23	**STT**
8.11	Beryllophosphate-H	**BPH**
8.15	Decamethonium DAF-1	**DFO**
8.15	ITQ-4, Calcined	**IFR**
8.15	Diethylamine Theta-1 (Silica ZSM-22)	**TON**

Powder Pattern Identification Table *continued*

2θ°	Material	Code
8.17	STA-1, Magnesium Aluminophosphate	SAO
8.20	Cobalt Gallium Phosphate-6	CGS
8.20	MAPO-36, Calcined	ATS
8.21	Partheite	-PAR
8.22	Ammonium Fluoride ZSM-23	MTT
8.32	Gottardiite	NES
8.32	Rho, Hydrated	RHO
8.37	NU-87	NES
8.49	Di-n-propylamine SAPO-31	ATO
8.56	Levyne	LEV
8.58	ITQ-3, Calcined	ITE
8.62	Terranovaite	TER
8.64	SAPO-56	AFX
8.64	RUB-13	RTH
8.68	1-aminoadamantane NU-3	LEV
8.71	SSZ-44, Calcined	SFF
8.72	RUB-17	RSN
8.73	STA-6	SAS
8.75	EU-1, Calcined, Rehydrated	EUO
8.81	Terranovaite	TER
8.81	ZSM-11, Calcined	MEL
8.82	GUS-1	GON
8.84	Tetrapropylammonium ZSM-5	MFI
8.87	VPI-7	VSV
8.88	Tetrapropylammonium ZSM-5	MFI
8.90	ZSM-5, Calcined	MFI
8.91	ZSM-12, Calcined	MTW
8.93	Rho, Deuterated Berylloarsenate	RHO
8.94	Lovdarite	LOV
8.95	Ammonium Fluoride ZSM-23	MTT
8.98	Maricopaite	MOR
9.01	ITQ-3, Calcined	ITE
9.01	1-aminoadamantane Sigma-2	SGT
9.05	RUB-13	RTH
9.07	Pahasapaite	RHO
9.08	AlPO-14, Calcined	AFN
9.10	CIT-1	CON
9.14	AlPO-C, Hydrated	APC
9.16	RUB-3	RTE
9.18	Quinuclidine AlPO-22	AWW
9.23	Ferrierite	FER
9.23	Cobalt Gallophosphate	LAU
9.24	Laumontite	LAU
9.28	UCSB-8Co	SBE
9.30	Tetramethylammonium OH AlPO-12	ATT
9.36	Magnesium STA-7	SAV
9.36	AlPO-25	ATV
9.38	Leonhardite	LAU
9.40	Chabazite	CHA
9.42	ZSM-57, SiO_2 Framework	MFS
9.42	Magnesium STA-7	SAV
9.43	SSZ-48, Calcined	SFE
9.45	Ferrierite, Siliceous	FER
9.45	Di-isopropylamine MnAPO-11	AEL
9.47	MAPO-39	ATN
9.47	(Cs,K) ZK5, Dehydrated	KFI
9.48	Methylbutylamine SAPO-47	CHA
9.49	AlPO-18, Calcined	AEI
9.49	Bellbergite	EAB
9.50	SSZ-23	STT

2θ°	Material	Code
9.54	AlPO-52, Calcined, Rehydrated	AFT
9.54	Perlialite	LTL
9.55	ZSM-18, SiO_2 Framework	MEI
9.57	AlPO-11, Calcined	AEL
9.59	VPI-8	VET
9.61	2-aminopentane Nonasil	NON
9.62	Mazzite	MAZ
9.64	(Na, Tetramethylammonium)-E	EAB
9.65	UiO-6, Calcined	OSI
9.65	Roggianite	-RON
9.68	Erionite	ERI
9.68	Beta, Polymorph A SiO_2 Framework	*BEA
9.69	Tschörtnerite	TSC
9.69	ITQ-4, Calcined	IFR
9.70	Stilbite	STI
9.71	Stellerite	STI
9.72	Barrerite	STI
9.72	AlPO-41, Calcined	AFO
9.73	SSZ-35, Calcined	STF
9.74	Li-LSX	FAU
9.75	MCM-35	MTF
9.75	Chiral Sodium Zincophosphate, $P6_122$	CZP
9.77	Mordenite	MOR
9.77	Piperidine AlPO-17	ERI
9.81	Chiral Sodium Zincophosphate, $P6_522$	CZP
9.81	Di-n-propylamine CoAPO-50	AFY
9.82	ERS-7 Framework	ESV
9.85	Heulandite	HEU
9.88	Clinoptilolite	HEU
9.90	Stellerite	STI
9.91	Barrerite	STI
9.95	Dachiardite	DAC
9.96	Stilbite	STI
9.97	Epistilbite	EPI
9.97	Na-X, Dehydrated	FAU
9.99	AlPO-8	AET
10.00	Cobalt Gallium Phosphate-5	CGF
10.00	Na-X, Hydrated	FAU
10.06	RUB-10, SiO_2 Framework	RUT
10.06	ITQ-3, Calcined	ITE
10.07	ASU-7	ASV
10.08	Tetramethylammonium ZAPO-M1	ZON
10.10	AlPO-21	AWO
10.12	OSB-1	OSO
10.14	AlPO-EN3	AEN
10.16	VPI-9	VNI
10.16	Diethylamine Theta-1 (Silica ZSM-22)	TON
10.17	Linde Type A, Hydrated	LTA
10.18	RUB-13	RTH
10.19	Linde Type A, Dehydrated	LTA
10.27	MCM-61	MSO
10.31	Na-Y, Siliceous	FAU
10.34	Ultrastable Y, Dehydrated Dealuminated	FAU
10.47	AlPO - H2	AHT
10.48	Magnesium STA-7	SAV
10.50	STA-6	SAS
10.58	SSZ-23	STT
10.61	AlPO-18, Calcined	AEI
10.70	Paulingite	PAU
10.75	Nepheline Hydrate	JBW

Powder Pattern Identification Table *continued*

2θ°	Material	Code
10.77	RUB-10, SiO_2 Framework	**RUT**
10.77	VPI-5	**VFI**
10.85	Levyne	**LEV**
10.90	Harmotome	**PHI**
10.90	Partheite	**-PAR**
11.07	Heulandite	**HEU**
11.08	1-aminoadamantane NU-3	**LEV**
11.11	Mazzite	**MAZ**
11.17	ZSM-18, SiO_2 Framework	**MEI**
11.19	Clinoptilolite	**HEU**
11.29	Bikitaite	**BIK**
11.30	Chiavennite	**-CHI**
11.33	Cobalt Gallium Phosphate-5	**CGF**
11.38	Chiral Sodium Zincophosphate, $P6_122$	**CZP**
11.41	Chiral Sodium Zincophosphate, $P6_522$	**CZP**
11.42	Li-LSX	**FAU**
11.43	Barium Chloroaluminosilicate	**MER**
11.45	Quinuclidine AlPO-16	**AST**
11.49	Cobalt Gallium Phosphate-6	**CGS**
11.52	Gmelinite	**GME**
11.53	Levyne	**LEV**
11.54	Losod	**LOS**
11.57	AlPO-14, Calcined	**AFN**
11.57	SAPO-56	**AFX**
11.64	AlPO-52, Calcined, Rehydrated	**AFT**
11.65	Offretite	**OFF**
11.67	Quinuclidinium fluoride octadecasil	**AST**
11.69	Na-X, Dehydrated	**FAU**
11.73	Na-X, Hydrated	**FAU**
11.77	Linde Type L	**LTL**
11.79	Nepheline Hydrate	**JBW**
11.86	Faujasite	**FAU**
11.86	Wenkite	**-WEN**
11.95	Magnesium Phosphate UiO-20	**DFT**
12.10	Na-Y, Siliceous	**FAU**
12.13	Amicite	**GIS**
12.14	Ultrastable Y, Dehydrated Dealuminated	**FAU**
12.15	Gismondine	**GIS**
12.22	AlPO-21	**AWO**
12.22	ACP-1	**ACO**
12.32	Cobalt Gallium Phosphate-6	**CGS**
12.35	Gobbinsite	**GIS**
12.36	Phillipsite	**PHI**
12.38	Garronite	**GIS**
12.38	Di-n-propylamine MAPO-43	**GIS**
12.40	Harmotome	**PHI**
12.41	Goosecreekite	**GOO**
12.42	Tetrapropylammonium SAPO-40	**AFR**
12.44	Merlinoite	**MER**
12.44	Tetramethylammonium ZAPO-M1	**ZON**
12.46	Na-P1	**GIS**
12.46	Linde Type A, Hydrated	**LTA**
12.48	Phillipsite	**PHI**
12.49	Linde Type A, Dehydrated	**LTA**
12.54	Merlinoite	**MER**
12.55	AlPO-C, Dehydrated	**APC**
12.57	Gobbinsite	**GIS**
12.58	Ferrierite, Siliceous	**FER**
12.59	Goosecreekite	**GOO**
12.60	ACP-1	**ACO**

2θ°	Material	Code
12.65	Tetramethylammonium OH AlPO-12	**ATT**
12.71	Laumontite	**LAU**
12.73	MCM-61	**MSO**
12.76	Franzinite	**FRA**
12.78	ZSM-57, SiO_2 Framework	**MFS**
12.78	Dachiardite	**DAC**
12.80	Maricopaite	**MOR**
12.83	Ferrierite, Siliceous	**FER**
12.84	Epistilbite	**EPI**
12.88	RUB-17	**RSN**
12.89	Methylbutylamine SAPO-47	**CHA**
12.90	AlPO-C, Hydrated	**APC**
12.91	Dodecasil 3C	**MTN**
12.91	AlPO-D	**APD**
12.91	AlPO-18, Calcined	**AEI**
12.99	AlPO-EN3	**AEN**
13.00	Leonhardite	**LAU**
13.07	Brewsterite	**BRE**
13.15	AlPO-14, Calcined	**AFN**
13.16	Lovdarite	**LOV**
13.17	Di-n-propylamine MAPSO-46	**AFS**
13.33	(Na, Tetramethylammonium)-E	**EAB**
13.34	Erionite	**ERI**
13.37	Scolecite	**NAT**
13.38	Piperidine AlPO-17	**ERI**
13.39	Thomsonite	**THO**
13.41	Montesommaite	**MON**
13.41	MAPO-39	**ATN**
13.41	Gonnardite	**NAT**
13.44	Mesolite	**NAT**
13.45	Mordenite	**MOR**
13.50	Bellbergite	**EAB**
13.56	Natrolite	**NAT**
13.60	Edingtonite	**EDI**
13.64	AlPO-C, Hydrated	**APC**
13.72	ITQ-4, Calcined	**IFR**
13.72	Losod	**LOS**
13.73	AlPO-41, Calcined	**AFO**
13.76	Tetramethylammonium ZAPO-M1	**ZON**
13.80	Li-ABW	**ABW**
13.88	RUB-17	**RSN**
13.89	STA-1, Magnesium Aluminophosphate	**SAO**
13.89	VPI-7	**VSV**
13.90	Harmotome	**PHI**
14.00	AlPO-C, Dehydrated	**APC**
14.02	Cancrinite	**CAN**
14.02	Brewsterite	**BRE**
14.14	RUB-3	**RTE**
14.16	Sodalite Octahydrate	**SOD**
14.31	Tugtupite	**SOD**
14.41	RUB-10, SiO_2 Framework	**RUT**
14.50	Roggianite	**-RON**
14.56	Partheite	**-PAR**
14.71	Linde Type L	**LTL**
14.74	Melanophlogite	**MEP**
14.80	AlPO-21	**AWO**
14.96	Gonnardite	**NAT**
14.96	AlPO-25	**ATV**
14.97	Weinebeneite	**WEI**
15.00	(Cs,K) ZK5, Dehydrated	**KFI**

Powder Pattern Identification Table *continued*

$2\theta^\circ$	Material	Code
15.04	Natrolite	**NAT**
15.10	Scolecite	**NAT**
15.10	N_2, Piperidine Dodecasil 1H	**DOH**
15.11	Mesolite	**NAT**
15.14	Dodecasil 3C	**MTN**
15.20	Chiavennite	**-CHI**
15.23	Ferrierite	**FER**
15.26	Chiral Sodium Zincophosphate, $P6_522$	**CZP**
15.27	Chiral Sodium Zincophosphate, $P6_122$	**CZP**
15.30	Yugawaralite	**YUG**
15.42	OSB-1	**OSO**
15.45	Weinebeneite	**WEI**
15.61	Faujasite	**FAU**
15.81	Analcime	**ANA**
16.16	Melanophlogite	**MEP**
16.24	STA-6	**SAS**
16.34	STA-2	**SAT**
16.42	STA-2	**SAT**
16.57	Merlinoite	**MER**
16.84	N_2, Piperidine Dodecasil 1H	**DOH**
17.13	1-aminoadamantane Deca-Dodecasil 3R	**DDR**
17.35	Amicite	**GIS**
17.65	Gmelinite	**GME**
17.82	Lovdarite	**LOV**
17.87	RUB-3	**RTE**
17.87	Garronite	**GIS**
17.90	AlPO–C, Dehydrated	**APC**
18.04	Gismondine	**GIS**
18.35	Liottite	**LIO**
18.40	Afghanite	**AFG**
18.54	Quinuclidine AlPO–22	**AWW**
18.61	Losod	**LOS**
18.67	Rho, Hydrated	**RHO**
18.75	Quinuclidine AlPO–16	**AST**
18.89	Edingtonite	**EDI**
19.06	MAPO–36, Calcined	**ATS**
19.15	Cancrinite	**CAN**
19.16	Yugawaralite	**YUG**
19.21	Thomsonite	**THO**
19.56	1-aminoadamantane Sigma-2	**SGT**
19.76	1-aminoadamantane Sigma-2	**SGT**
19.82	Goosecreekite	**GOO**
20.01	Moganite	–
20.08	CIT-5	**CFI**
20.09	VPI-8	**VET**
20.18	Di-n-propylamine SAPO–31	**ATO**
20.34	Gottardiite	**NES**
20.36	Diethylamine Theta-1 (Silica ZSM-22)	**TON**
20.45	Chabazite	**CHA**
20.52	Tridymite	–
20.53	EU-1, Calcined, Rehydrated	**EUO**
20.58	Tridymite	–
20.61	Quinuclidine AlPO–22	**AWW**
20.62	2-aminopentane Nonasil	**NON**
20.62	AlPO–D	**APD**
20.62	Methylbutylamine SAPO–47	**CHA**
20.64	UiO-6, Calcined	**OSI**
20.66	GUS-1	**GON**
20.71	AlPO–D	**APD**
20.82	Gismondine	**GIS**

$2\theta^\circ$	Material	Code
20.86	Alpha Quartz	–
20.96	UTD-1	**DON**
20.97	Tetrapropylammonium Fluoride AlPO-5	**AFI**
21.03	Amicite	**GIS**
21.04	Di-isopropylamine MnAPO–11	**AEL**
21.10	Barium Chloroaluminosilicate	**MER**
21.13	AlPO–25	**ATV**
21.18	Cobalt Gallophosphate	**LAU**
21.22	Bikitaite	**BIK**
21.23	AlPO–11, Calcined	**AEL**
21.52	Di-n-propylamine MAPO–43	**GIS**
21.52	STA-2	**SAT**
21.57	Gobbinsite	**GIS**
21.60	Cs-Aluminosilicate	**CAS**
21.67	Na-P1	**GIS**
21.68	Tridymite	–
21.87	AlPO - H2	**AHT**
21.89	Stilbite	**STI**
21.90	Stellerite	**STI**
21.92	Barrerite	**STI**
22.00	Alpha Cristobalite	–
22.03	1-aminoadamantane NU-3	**LEV**
22.03	Quinuclidine AlPO–16	**AST**
22.13	Quinuclidinium fluoride octadecasil	**AST**
22.22	Heulandite	**HEU**
22.38	Tetrapropylammonium Fluoride AlPO-5	**AFI**
22.49	Clinoptilolite	**HEU**
22.52	Perlialite	**LTL**
22.58	Di-n-propylamine SAPO–31	**ATO**
22.59	MAPO–39	**ATN**
22.60	VPI-5	**VFI**
22.62	Quinuclidinium fluoride octadecasil	**AST**
22.65	ASU-7	**ASV**
22.96	Epistilbite	**EPI**
23.05	Boggsite	**BOG**
23.11	Cobalt Gallium Phosphate-5	**CGF**
23.13	ZSM-11, Calcined	**MEL**
23.24	Magnesium Phosphate UiO-20	**DFT**
23.48	ASU-7	**ASV**
23.53	Offretite	**OFF**
23.57	(Na, Tetramethylammonium)-E	**EAB**
23.78	Rho, Deuterated Berylloarsenate	**RHO**
23.86	Keatite	–
23.86	Franzinite	**FRA**
23.95	Liottite	**LIO**
23.96	AlPO-EN3	**AEN**
24.08	Afghanite	**AFG**
24.16	Pahasapaite	**RHO**
24.18	Di-n-propylamine CoAPO–50	**AFY**
24.65	Sodalite Octahydrate	**SOD**
24.68	Cs-Aluminosilicate	**CAS**
24.71	Bicchulite	**SOD**
24.79	Edingtonite	**EDI**
24.79	Melanophlogite	**MEP**
24.80	Tugtupite	**SOD**
24.83	Cs-Aluminosilicate	**CAS**
25.14	Tugtupite	**SOD**
25.14	Rho, Hydrated	**RHO**
25.18	Laumontite	**LAU**
25.19	Cobalt Gallophosphate	**LAU**

Powder Pattern Identification Table *continued*

$2\theta^\circ$	Material	Code
25.37	Leonhardite	LAU
25.42	Thomsonite	THO
25.59	MCM-35	MTF
25.73	Dachiardite	DAC
25.76	Bikitaite	BIK
25.77	Wenkite	-WEN
25.96	Analcime	ANA
26.03	Keatite	–
26.07	Magnesium Phosphate UiO-20	DFT
26.10	Nepheline Hydrate	JBW
26.29	Moganite	–
26.49	Tiptopite	CAN
26.65	Alpha Quartz	–
26.73	Moganite	–
26.73	Keatite	–
26.91	Liottite	LIO
27.01	Montesommaite	MON
27.02	Afghanite	AFG
27.02	Rho, Deuterated Berylloarsenate	RHO
27.43	VPI-7	VSV
27.46	Pahasapaite	RHO
27.54	Tetramethylammonium OH AlPO-12	ATT
27.66	Di-n-propylamine MAPO-43	GIS
27.72	ACP-1	ACO
27.74	Cancrinite	CAN
27.89	Phillipsite	PHI
28.10	Na-P1	GIS

$2\theta^\circ$	Material	Code
28.15	Li-ABW	ABW
28.33	Garronite	GIS
28.37	Wenkite	-WEN
28.42	Montesommaite	MON
29.03	AlPO - H2	AHT
29.10	VPI-9	VNI
29.29	Yugawaralite	YUG
29.36	OSB-1	OSO
29.50	Li-ABW	ABW
30.19	Tiptopite	CAN
30.40	Chabazite	CHA
30.50	Brewsterite	BRE
30.54	Analcime	ANA
30.96	Scolecite	NAT
30.98	Mesolite	NAT
31.01	Gonnardite	NAT
31.22	Natrolite	NAT
31.44	Alpha Cristobalite	–
31.99	Sodalite Octahydrate	SOD
32.07	Bicchulite	SOD
32.08	Beryllophosphate-H	BPH
32.32	Barium Chloroaluminosilicate	MER
35.58	Tiptopite	CAN
35.73	Weinebeneite	WEI
36.15	Alpha Cristobalite	–
39.49	Alpha Quartz	–
43.51	Bicchulite	SOD